Modeling Atmospheric Impacts of Point Source Carbon Capture

Workshop on Measurement, Monitoring and Controlling Potential Environmental Impacts from the Installation of Point Source Capture

Eladio Knipping, Ph.D., EPRI,
eknipping@epri.com

Prakash Karamchandani, Ph.D., Ramboll,
pkaramchandani@ramboll.com

June 8, 2023

Background

- Emissions of “traditional” air pollutants (criteria air pollutants), amines and amine byproducts during carbon capture may have an adverse impacts on human health and the environment.
  - **Are they significant compared to current air quality impacts?**
  - **How do predicted concentrations compare to levels of concern?**

- Emissions and Chemistry
  - Traditional emissions (NOx, SOx, …)
  - Direct emissions of amines and byproducts (nitrosamines and nitramines) formed within the carbon capture system

- Chemistry
  - Formation of ozone and fine particulate matter
  - Formation of harmful pollutants from the atmospheric chemistry of emitted amines:
    - Nitrosamines and nitramines
    - Isocyanic acid (HNCO)

- **Modeling atmospheric impacts of these emissions requires the use of dispersion models that can handle complex atmospheric chemistry**

Notes

- Although this presentation focuses on amine chemistry, it is important to note that it is critical to continue to model the traditional pollutants

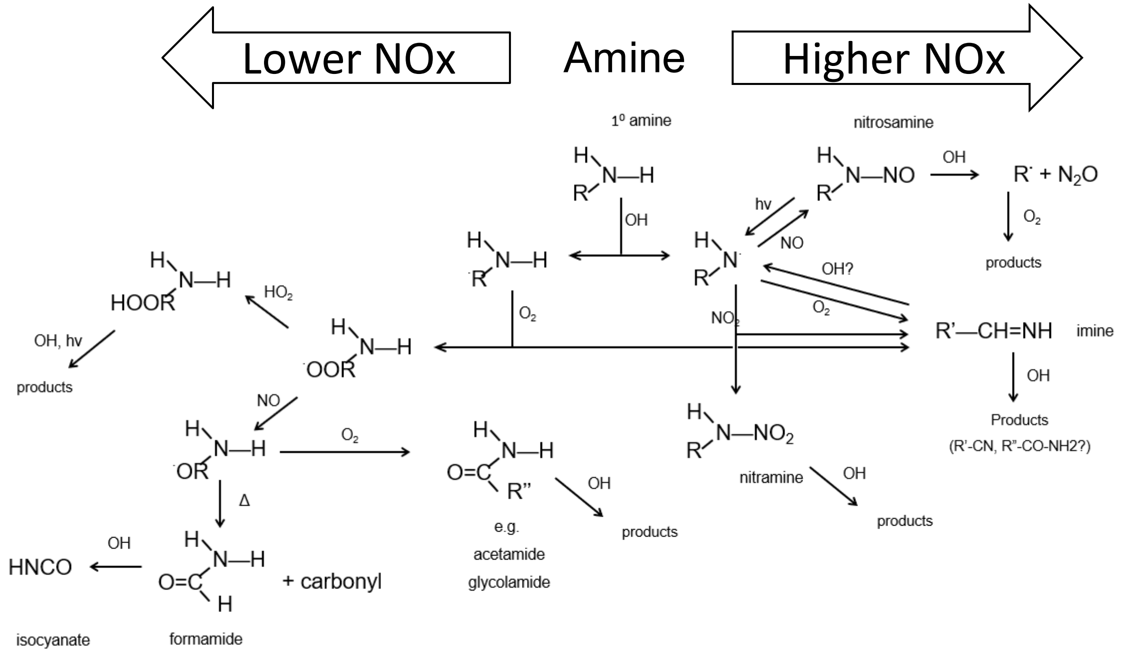
- It is also critical to have a representation of the chemical composition of the background onto which the emissions from carbon capture systems are released

EPRI

Atmospheric Chemistry of Amines

- Amines react in the gas-phase with OH radical and other oxidants
  - Identity and amounts of products formed depend on NOx concentration
  - Nitrosamines and nitramines tend to form with high NOx
  - Isocyanic acid tends to form with low NOx
  - Nitrosamines can photolyze back to the amino radical
- Amines form particles with sulfuric acid and nitric acid (a potential sink for amines)
- Some amine reaction products can form secondary organic aerosols (SOA)

OH Reaction Scheme for Primary (1º) Amines



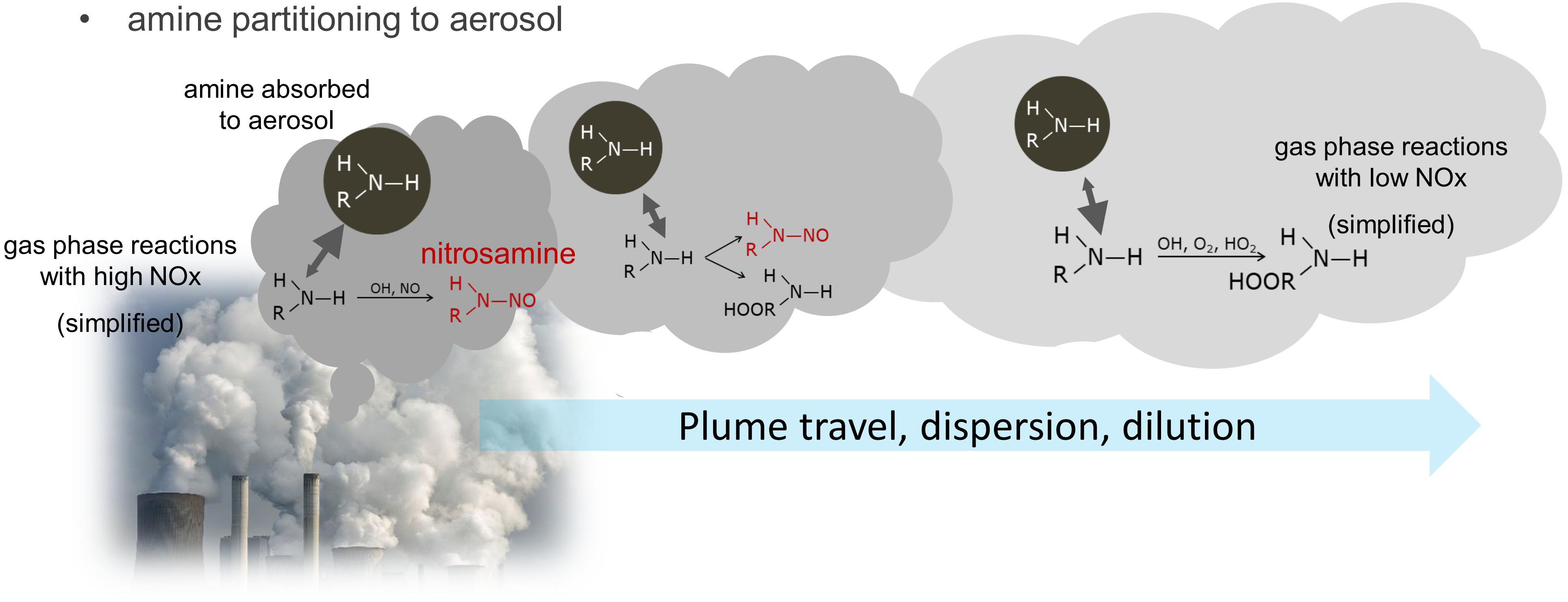
Gas and Aerosol Chemistry Interact to Change Amine Degradation Products

Near source

- low dilution
- "high NOx" degradation products
- amine partitioning to aerosol

Downwind

- high dilution
- "low NOx" degradation products
- amine evaporation from aerosol



Amines of Interest

Amine	k_{OH} (Rate constant for OH reaction), cm^3 $molecule^{-1}$ s^{-1}
Monoethanolamine (MEA)	4.41×10^{-11} to $(9.2 \pm 1.1) \times 10^{-11}$
Dimethylethanolamine (DMEA)	$(4.7 \pm 1.2) \times 10^{-11}$ to $(9.0 \pm 2.0) \times 10^{-11}$
Monomethylethanolamine (MMEA)	$(8.51 \pm 0.65) \times 10^{-11} (T/298)^{-(0.79 \pm 0.22)}$
2-Amino-2-methylpropanol (AMP)	$(2.8 \pm 0.5) \times 10^{-11}$ to $5.2 \times 10^{-12} \times \exp(505/T)$
Piperazine (PZ)	1.3×10^{-10} to $(2.8 \pm 0.6) \times 10^{-10}$

Examples of Previous MEA Modeling Studies

- Box Models:
  - Karl, M., Dye, C., Schmidbauer, N., Wisthaler, A., Mikoviny, T., D'Anna, B., et al. (2012). Study of OH-initiated degradation of 2-aminoethanol. Atmos. Chem. Phys., 12(4), 1881-1901.
  - Onel, L., Blitz, M. A., Breen, J., Rickard, A. R., & Seakins, P. W. (2015). Branching ratios for the reactions of OH with ethanol amines used in carbon capture and the potential impact on carcinogen formation in the emission plume from a carbon capture plant. [10.1039/C5CP04083C]. Physical Chemistry Chemical Physics, 17(38), 25342-25353.

- Gaussian Dispersion Model:
  - Manzoor, S., Korre, A., Durucan, S., & Simperler, A. (2014). Atmospheric Chemistry Modelling of Amine Emissions from Post Combustion CO_2 Capture Technology. Energy Procedia, 63, 822-829.

- Eulerian Grid Models:
  - Karl, M., Castell, N., Simpson, D., Solberg, S., Starrfelt, J., Svendby, T., Walker, S.-E., and Wright, R. F. (2014). Uncertainties in assessing the environmental impact of amine emissions from a CO_2 capture plant, Atmos. Chem. Phys., 14, 8533–8557.
  - Karl, M., Svendby, T., Walker, S. E., Velken, A. S., Castell, N., & Solberg, S. (2015). Modelling atmospheric oxidation of 2-aminoethanol (MEA) emitted from post-combustion capture using WRF–Chem. Science of The Total Environment, 527-528, 185-202.

Dispersion Models Considered for this Study

Steady-State Gaussian Models (e.g., EPA AERMOD)	Non-Steady-State Puff Model with Chemistry (SCICHEM)
Constant and horizontally homogeneous meteorological conditions for a modeling interval (typically 1 hour)	3-D time varying meteorology
Straight line trajectories for a modeling interval	More realistic plume behavior with 3-D puffs traveling in different directions
Simplified dispersion treatment	Second-order closure for dispersion
Generally single-pollutant models (no chemistry). For Gaussian models that include some chemical reactions, the chemistry terms are parameterized and reduced to first-order (linear) chemistry	Multiple pollutants with explicit non-linear chemistry treatment. Chemistry in overlapping puffs to correctly account for interaction among puffs and with background-allows treatment of non-linear chemistry
Not suitable for distances > 50 km	Suitable for both near-field and far-field impacts
Computationally economical with minimal resource requirements	Computationally more expensive than steady-state Gaussian models, but less resource-intensive than Eulerian (fixed grid) models with full chemistry

Dispersion Model Selection

- SCICHEM selected for modeling amine impacts:
  - Model both near-source impacts (EJ considerations) and far-source impacts of amines and products
  - Model traditional pollutants typically emitted from combustion sources with carbon capture systems (SO_2, NOx, particulate matter, ammonia)
  - Explicit non-linear chemistry treatment to model amine gas-phase chemistry, including chemistry leading to O_3 and OH formation (NOx and VOC chemistry)
  - Model aerosol (particulate matter) chemistry
  - Efficiently model a large number of scenarios
  - Open-source model, distributed freely to the air quality modeling community by EPRI

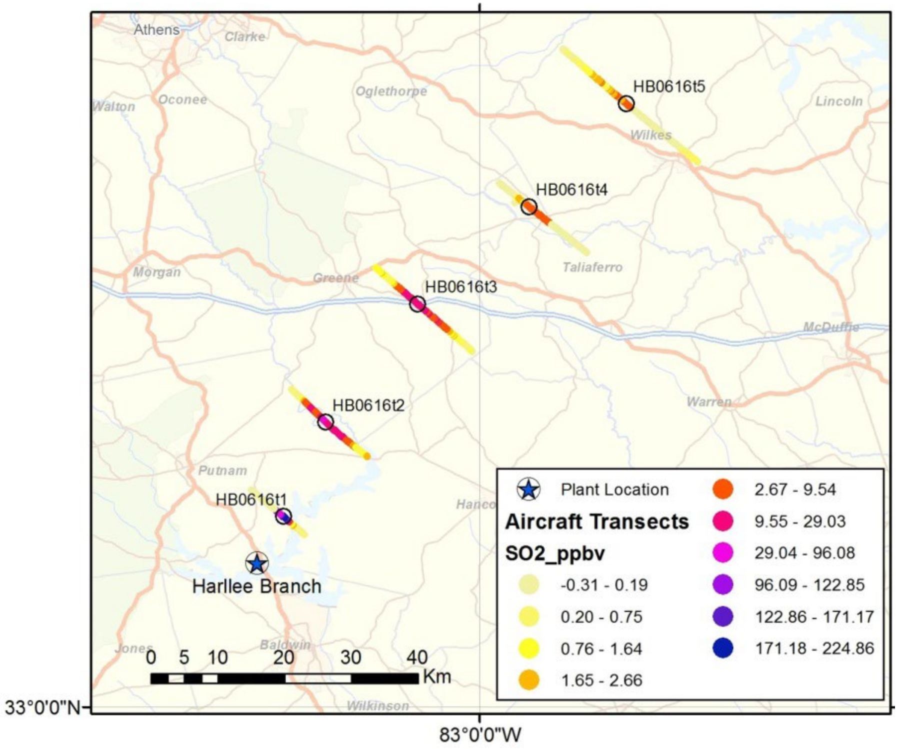
Model Inputs

- Emissions
  - Chemical speciation and mass flow rates
- Stack Parameters
  - Height/diameter
  - Temperature
  - Velocity
- Meteorology
- Surroundings
  - Location
  - Terrain and buildings
  - Chemical background* (background concentrations of other ambient species)

- The critical piece to our study will be characterizing the emissions.
- We can make assumptions, but with actual emissions rates our simulations can better approximate impacts to multiple locations

Harllee Branch Power Plant Plume, June 16, 2013

Aircraft Transects

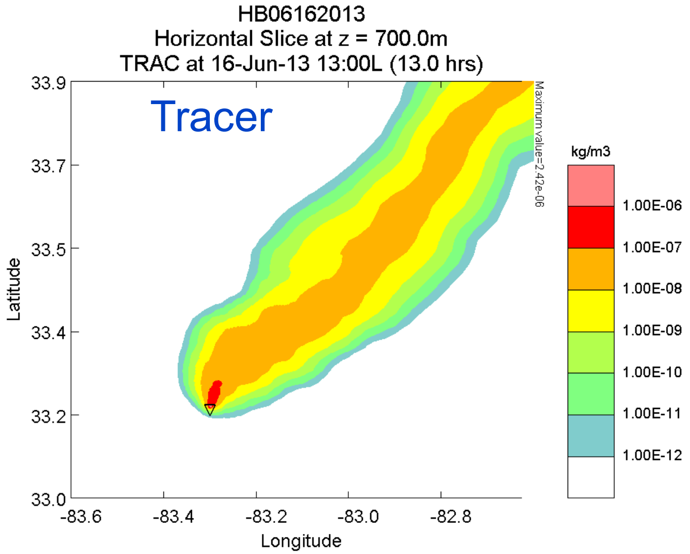


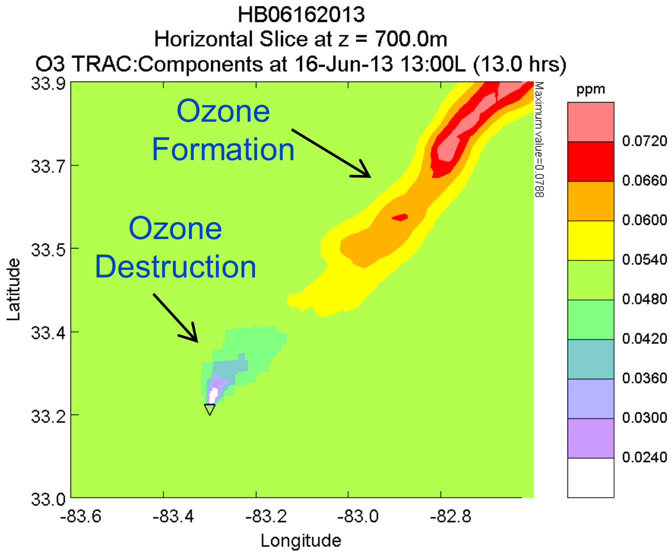
Aircraft Altitudes: 680 to 800 m (MSL)

Sampling Times: 12:45 pm to 3:45 pm LST

Emissions: 165 TPD SO_2, 140 TPD NOx

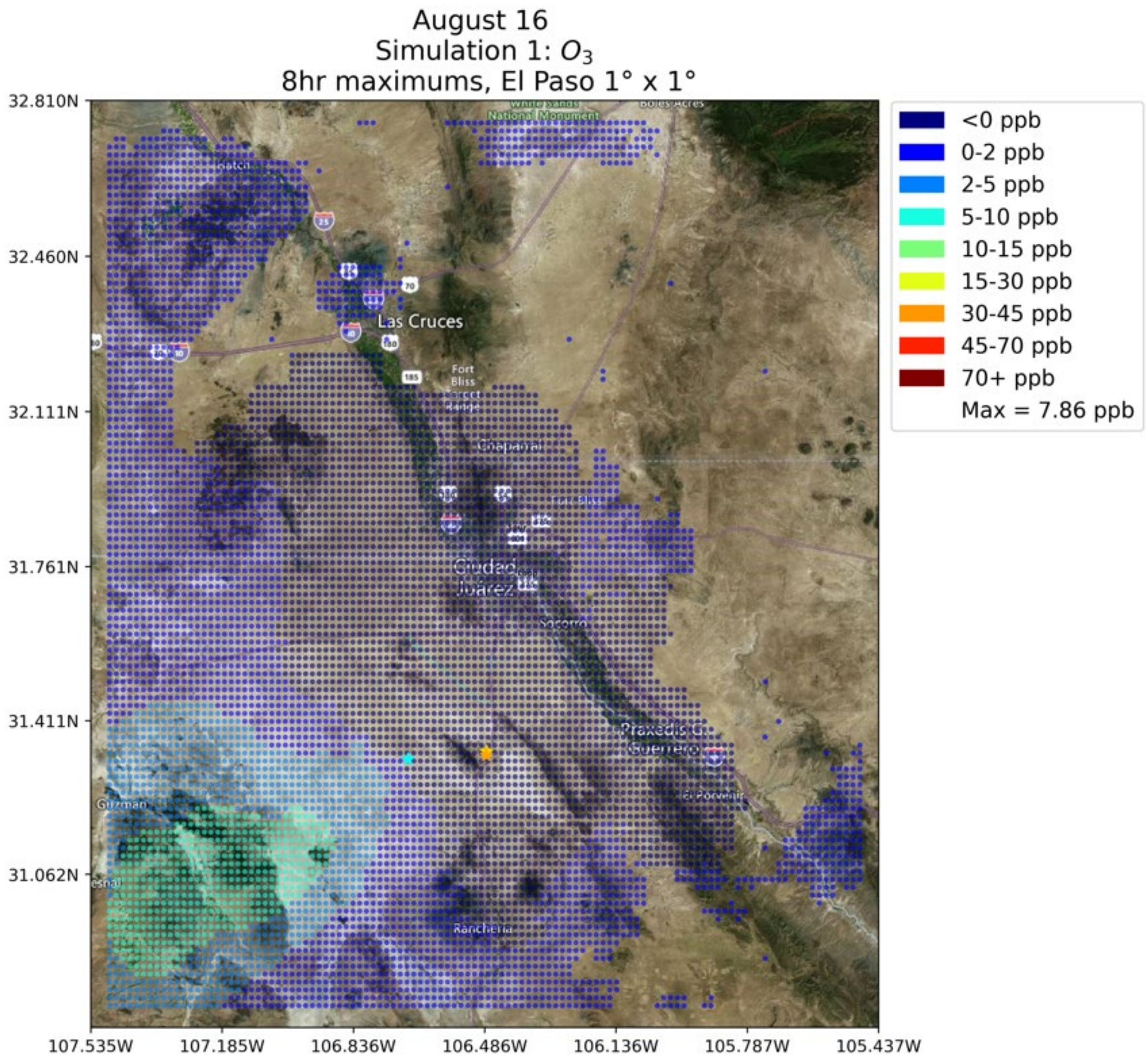
SCICHEM Plume





Ozone Contribution from Mexican EGUs

(SCICHEM study sponsored by TCEQ)



Conclusions

- Currently conducting a study to evaluate atmospheric impacts of point source carbon capture
  - Applying the SCICHEM **photochemical** dispersion model
  - Enhancing SCICHEM to incorporate amine chemistry
  - Will conduct case studies for various conditions, including different background concentrations
  - Will benefit from knowledge from carbon capture experts at EPRI to bound emissions scenarios
  - **The broader the collaboration, the more value we can obtain from this study**